



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:03 PM BST

PDB ID : 4V76  
EMDB ID: : EMD-1722  
Title : E. coli 70S-fMetVal-tRNAVal-tRNA<sup>f</sup>Met complex in intermediate post-translocation state (post2a)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 17.00 Å(reported)  
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

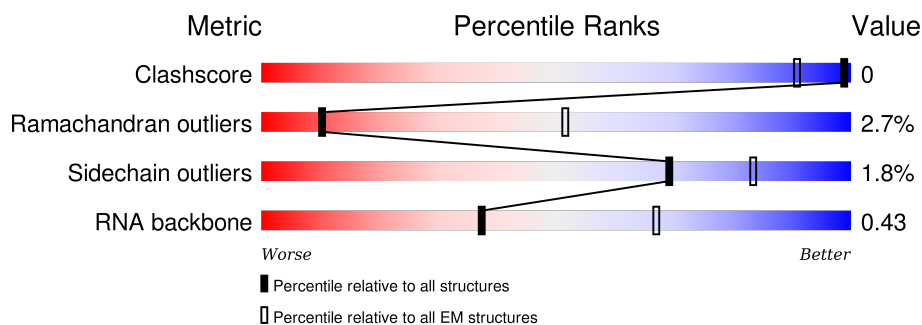
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 17.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.














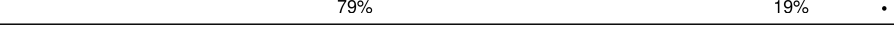
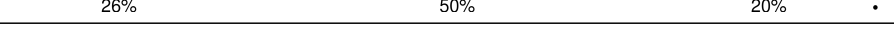


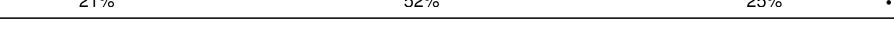



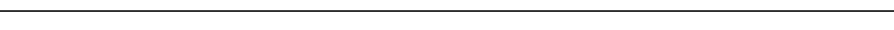

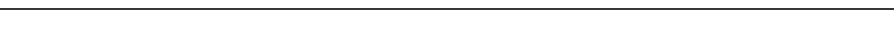
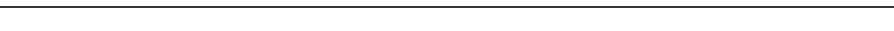


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AB	220	91% 9%
2	AC	208	90% 9%
3	AD	206	89% 10% .
4	AE	152	91% 9%
5	AF	101	87% 13%
6	AG	152	86% 14% .
7	AH	130	91% 8% .
8	AI	128	90% 9% .













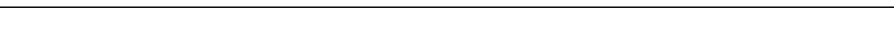



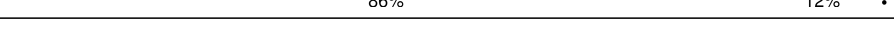




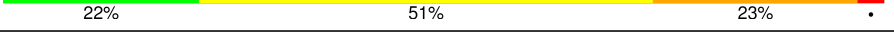
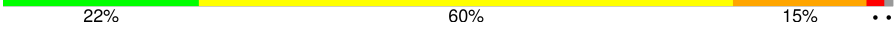
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Mol	Chain	Length	Quality of chain
9	AJ	100	 85% 13% .
10	AK	118	 89% 9% .
11	AL	124	 81% 16% ..
12	AM	115	 82% 17% .
13	AN	101	 82% 17% .
14	AO	89	 82% 17% .
15	AP	81	 86% 14%
16	AQ	82	 90% 10%
17	AR	57	 86% 14%
18	AS	81	 85% 15%
19	AT	86	 92% 8%
20	AU	53	 79% 19% .
21	AA	1533	 26% 50% 20% .
22	A1	76	 32% 51% 13% .
23	A2	15	 13% 47% 27% 13%
24	A3	77	 21% 52% 25% .
25	BC	273	 86% 14%
26	BD	209	 91% 8%
27	BE	201	 91% 9%
28	BF	179	 89% 9% ..
29	BG	177	 93% 6% ..
30	BH	149	 94% 6%
31	BI	142	 95% . .
32	BJ	142	 90% 9% .
33	BK	123	 85% 13% .

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Mol	Chain	Length	Quality of chain
34	BL	144	 86% 13% .
35	BM	136	 90% 10%
36	BN	121	 85% 15%
37	BO	117	 88% 11% .
38	BP	115	 85% 12% ..
39	BQ	118	 84% 14% ..
40	BR	103	 93% 7%
41	BS	110	 91% 9%
42	BT	94	 89% 11%
43	BU	104	 85% 13% ..
44	BV	94	 94% 6%
45	BW	80	 79% 18% .
46	BX	79	 84% 13% ..
47	BY	63	 89% 11%
48	BZ	59	 88% 8% ..
49	B0	57	 86% 12% .
50	B1	52	 92% 6% .
51	B2	46	 76% 22% .
52	B3	65	 80% 18% .
53	B4	38	 84% 16%
54	BA	2903	 22% 51% 23% .
55	BB	118	 22% 60% 15% ..
56	B5	234	 88% 7% 5%

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	ACETYLATION	UNP P0A7V0
AB	226	NH2	-	AMIDATION	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	AMIDATION	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total	C	N	O	S	0	1
			1109	689	212	202	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	ACETYLATION	UNP P0A7W1
AE	159	NH2	-	AMIDATION	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	AMIDATION	UNP P02358

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total	C	N	O	S	0	1
			1178	732	227	215	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	ACETYLATION	UNP P02359
AG	152	NH2	-	AMIDATION	UNP P02359

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total	C	N	O	S	0	0
			1025	636	206	180	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	ACETYLATION	UNP P0A7X3

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total	C	N	O	S	0	1
			790	495	151	143	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	ACETYLATION	UNP P0A7R5
AJ	103	NH2	-	AMIDATION	UNP P0A7R5

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total	C	N	O	S	0	0
			880	542	174	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	ACETYLATION	UNP P0A7R9

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	114	Total	C	N	O	S	0	1
			877	541	178	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	AMIDATION	UNP P0A7S9

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	81	Total	C	N	O	S	0	1
			639	400	127	111	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	AMIDATION	UNP P0A7T3

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1
			652	413	122	114	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	ACETYLATION	UNP P0AG63
AQ	83	NH2	-	AMIDATION	UNP P0AG63

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AR	57	Total	C	N	O	0	1
			459	290	87	82		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	18	ACE	-	ACETYLATION	UNP P0A7T7

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	AMIDATION	UNP P0A7T7

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total	C	N	O	S	0	1
			641	410	121	108	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	ACETYLATION	UNP P0A7U3
AS	81	NH2	-	AMIDATION	UNP P0A7U3

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	86	Total	C	N	O	S	0	0
			668	413	137	115	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	ACETYLATION	UNP P0A7U7

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total	C	N	O	S	0	1
			429	267	87	74	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	ACETYLATION	UNP P68679
AU	54	NH2	-	AMIDATION	UNP P68679

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32828	14642	6024	10633	1529		

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

- Molecule 23 is a RNA chain called 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*P\*AP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P	0	0
			309	140	46	109	14		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1642	734	297	534	76	1		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	272	NH2	-	AMIDATION	UNP P60422

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	123	Total	C	N	O	S	0	1
			939	587	181	165	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	123	NH2	-	AMIDATION	UNP P0ADY3

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	121	Total	C	N	O	S	0	1
			961	593	197	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	121	NH2	-	AMIDATION	UNP P0AG44

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BO	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BQ	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	94	Total	C	N	O	S	0	1
			739	466	140	131	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	94	NH2	-	AMIDATION	UNP P0ADZ0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BU	103	Total	C	N	O	0	1
			780	492	147	141		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	103	NH2	-	AMIDATION	UNP P60624

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	80	Total	C	N	O	S	0	0
			599	369	120	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	5	ACE	-	ACETYLATION	UNP P0A7L8

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	-1	ACE	-	ACETYLATION	UNP P0A7M2

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	B1	52	Total	C	N	O	0	1
			413	265	76	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	ACETYLATION	UNP P0A7N9
B1	53	NH2	-	AMIDATION	UNP P0A7N9

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BA	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

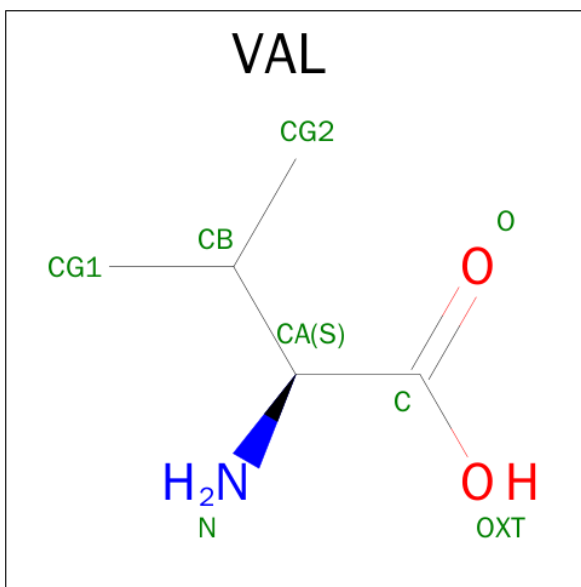
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BB	117	Total	C	N	O	P	0	0
			2504	1116	459	813	116		

- Molecule 56 is a protein called 50S ribosomal protein L1.

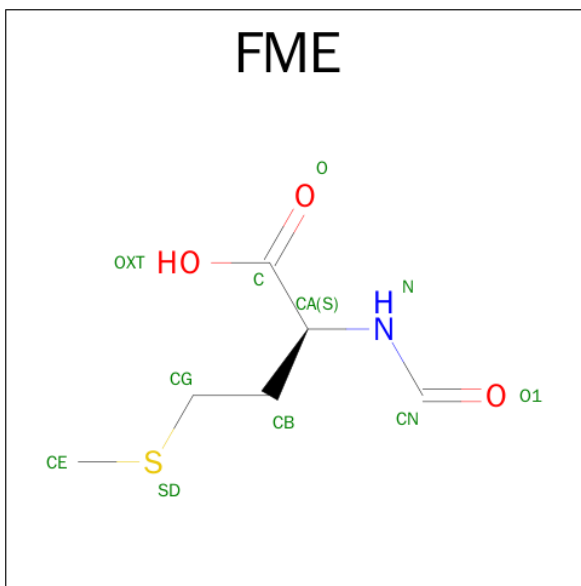
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
57	A1	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



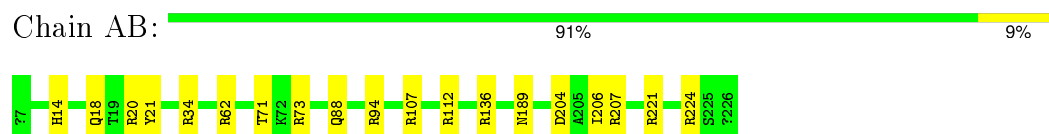
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



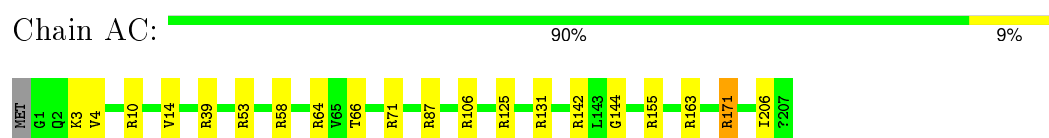
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

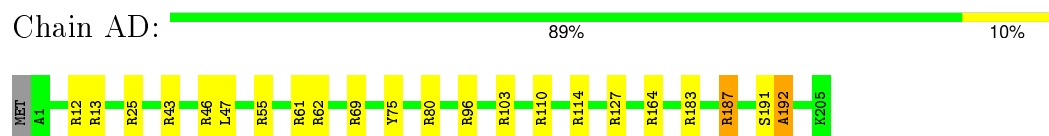
- Molecule 1: 30S ribosomal protein S2



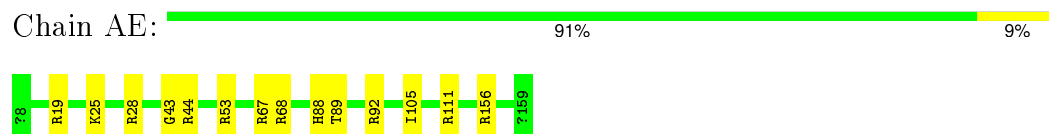
- Molecule 2: 30S ribosomal protein S3



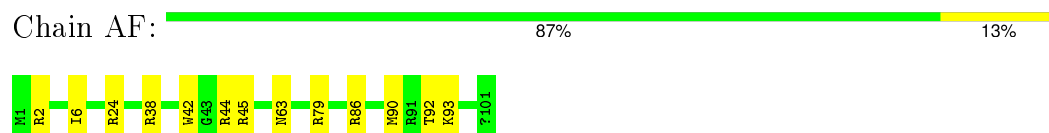
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





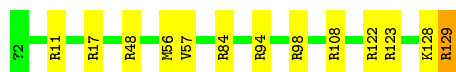
- Molecule 7: 30S ribosomal protein S8

Chain AH: 91% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 90% 9%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 85% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 89% 9%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 81% 16%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 82% 17%




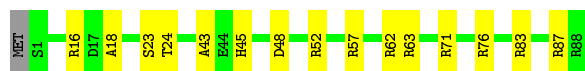
- Molecule 13: 30S ribosomal protein S14

Chain AN: 82% 17%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  82% 17%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  86% 14%




- Molecule 16: 30S ribosomal protein S17

Chain AQ:  90% 10%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  86% 14%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  85% 15%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  92% 8%



- Molecule 20: 30S ribosomal protein S21

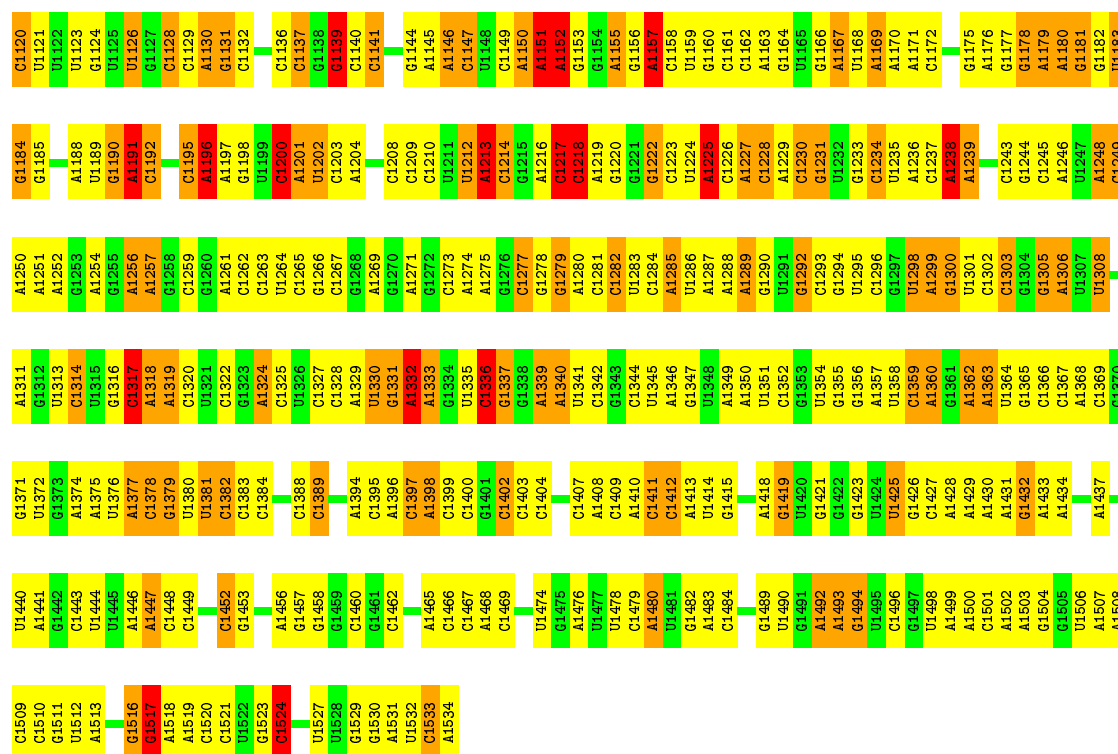
Chain AU:  79% 19%



- Molecule 21: 16S ribosomal RNA

Chain AA:  26% 50% 20%

C1051	U1052	C1053	C1054	C1055	U1056	C1059	U1060	C1061	U1062	C1063	C1064	U1065	C1066	A1067	C1068	U1069	C1070	C1071	U1072	C1073	U1074	C1075	U1076	C1077	A1080	A1081	U1082	U1083	A1092	A1093	C1094	U1095	C1096	C1097	C1098	U1099	C1100	C1101	A1102	C1103	C1104	A1105	C1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113	C1114	U1115	U1116	A1117	U1118	C1119																																																																					
G985	U986	C989	C990	C991	U992	G993	A994	C995	A996	U997	C998	C999	A1000	C1001	G1002	C1003	A1004	A1005	C1010	C1011	U1012	U1013	A1014	G1015	A1016	U1017	G1018	A1019	U1020	A1021	A1022	U1023	C1026	C1027	C1028	U1029	U1030	C1031	G1032	G1033	C1034	A1035	A1036	C1037	C1038	G1041	A1042	G1043	C1044	C1045	U1046	U1047	C1048	U1049	C1050																																																																						
G719	C720	G721	G722	U723	G724	G725	G726	G727	A728	U729	C732	C735	C736	C737	C738	U739	U740	A807	C808	G809	A742	A675	A676	C679	C680	A681	A682	A683	A687	G688	C689	G690	G691	A694	A695	A696	U697	G698	C699	G700	U701	A702	G703	A704	G705	A706	U707	C708	U709	G710	G711	A712	G713	G714	A715	A716	A717	A718																																																																			
G786	A787	U788	U789	A790	G791	U792	U793	A794	C795	C796	C797	G800	U801	A802	G803	U804	C805	C806	A807	C808	G809	A742	A675	A676	C679	C680	A681	A682	A683	A687	G688	C689	G690	G691	A694	A695	A696	U697	G698	C699	G700	U701	A702	G703	A704	G705	A706	U707	C708	U709	G710	G711	A712	G713	G714	A715	A716	A717	A718																																																																		
C857	G858	G859	A860	G861	C862	U863	A864	A865	C866	U867	C868	C869	U870	U871	A872	C873	A874	U875	C876	G877	A878	C879	C880	C881	C882	C883	U884	A885	A886	C887	C888	A889	G890	U891	A892	C893	U894	G895	C896	C897	U898	A900	A901	G902	C903	C904	U904	U905	A906	A907	A908	A909	C910	U911	C912	A913	A914	U915	U916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	A983	C984
G917	A918	A919	U920	G921	C922	A923	C924	G925	A926	G927	C930	C931	U932	C933	A934	C935	A936	A937	A938	G939	C940	G941	G944	G945	A946	G947	C948	A949	G954	U957	A958	A959	U960	U961	C962	G963	A964	U965	C966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	A978	A979	C980	A983	C984																																																																						
C985	U986	U989	C990	U991	U992	G993	A994	C995	A996	U997	C998	C999	A1000	C1001	G1002	C1003	A1004	A1005	U1010	C1011	U1012	U1013	A1014	G1015	A1016	U1017	G1018	A1019	U1020	A1021	A1022	U1023	G1026	C1027	C1028	U1029	U1030	C1031	G1032	G1033	C1034	A1035	A1036	C1037	C1038	G1041	A1042	G1043	C1044	C1045	U1046	U1047	C1048	U1049	C1050																																																																						
A65	A66	C67	G68	A71	A72	C73	A74	G75	G76	A77	U78	G79	A80	A81	G82	C83	U84	U85	G86	C87	U88	U89	C90	G94	G95	U96	G97	A98	C99	G100	A101	G105	G106	G107	G108	A109	C110	G111	G112	G113	U114	G115	A116	G117	U118	A119	A120	U121	G122	U123	C124	A129	A130	A131	C132																																																																						



• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 32% 51% 13%



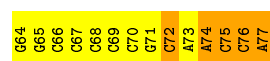
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

Chain A2: 13% 47% 27% 13%



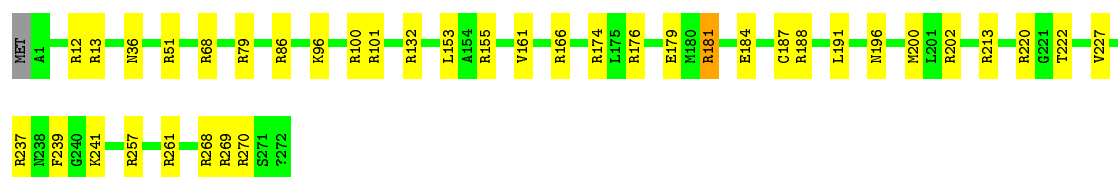
• Molecule 24: tRNA-fMet

Chain A3: 21% 52% 25%



• Molecule 25: 50S ribosomal protein L2

Chain BC: 86% 14%



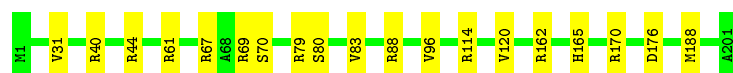
- Molecule 26: 50S ribosomal protein L3

Chain BD: 91% 8%



- Molecule 27: 50S ribosomal protein L4

Chain BE: 91% 9%



- Molecule 28: 50S ribosomal protein L5

Chain BF: 89% 9% ..



- Molecule 29: 50S ribosomal protein L6

Chain BG: 93% 6% ..



- Molecule 30: 50S ribosomal protein L9

Chain BH: 94% 6%



- Molecule 31: 50S ribosomal protein L11

Chain BI: 95% ..



- Molecule 32: 50S ribosomal protein L13

Chain BJ: 90% 9% .



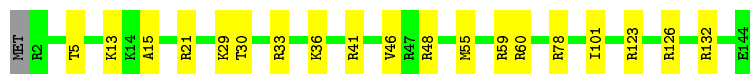
- Molecule 33: 50S ribosomal protein L14

Chain BK: 85% 13%



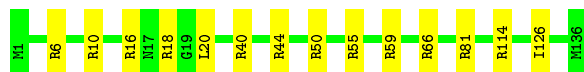
- Molecule 34: 50S ribosomal protein L15

Chain BL: 86% 13%



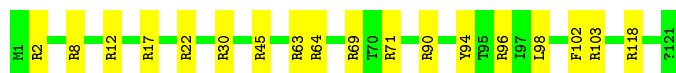
- Molecule 35: 50S ribosomal protein L16

Chain BM: 90% 10%



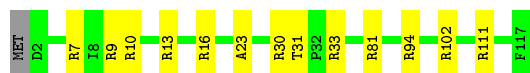
- Molecule 36: 50S ribosomal protein L17

Chain BN: 85% 15%



- Molecule 37: 50S ribosomal protein L18

Chain BO: 88% 11%



- Molecule 38: 50S ribosomal protein L19

Chain BP: 85% 12%



- Molecule 39: 50S ribosomal protein L20

Chain BQ: 84% 14%



- Molecule 40: 50S ribosomal protein L21

Chain BR:  93% 7%



- Molecule 41: 50S ribosomal protein L22

Chain BS:  91% 9%




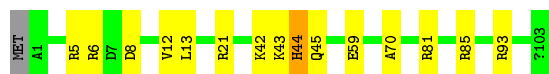
- Molecule 42: 50S ribosomal protein L23

Chain BT:  89% 11%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  85% 13% ..




- Molecule 44: 50S ribosomal protein L25

Chain BV:  94% 6%




- Molecule 45: 50S ribosomal protein L27

Chain BW:  79% 18% .



- Molecule 46: 50S ribosomal protein L28

Chain BX:  84% 13% ..




- Molecule 47: 50S ribosomal protein L29



Chain BY:  89% 11%




- Molecule 48: 50S ribosomal protein L30

Chain BZ:  88% 8% ..



- Molecule 49: 50S ribosomal protein L32

Chain B0:  86% 12% .




- Molecule 50: 50S ribosomal protein L33

Chain B1:  92% 6% .




- Molecule 51: 50S ribosomal protein L34

Chain B2:  76% 22% .




- Molecule 52: 50S ribosomal protein L35

Chain B3:  80% 18% .

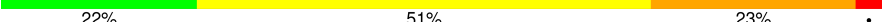


- Molecule 53: 50S ribosomal protein L36

Chain B4:  84% 16%

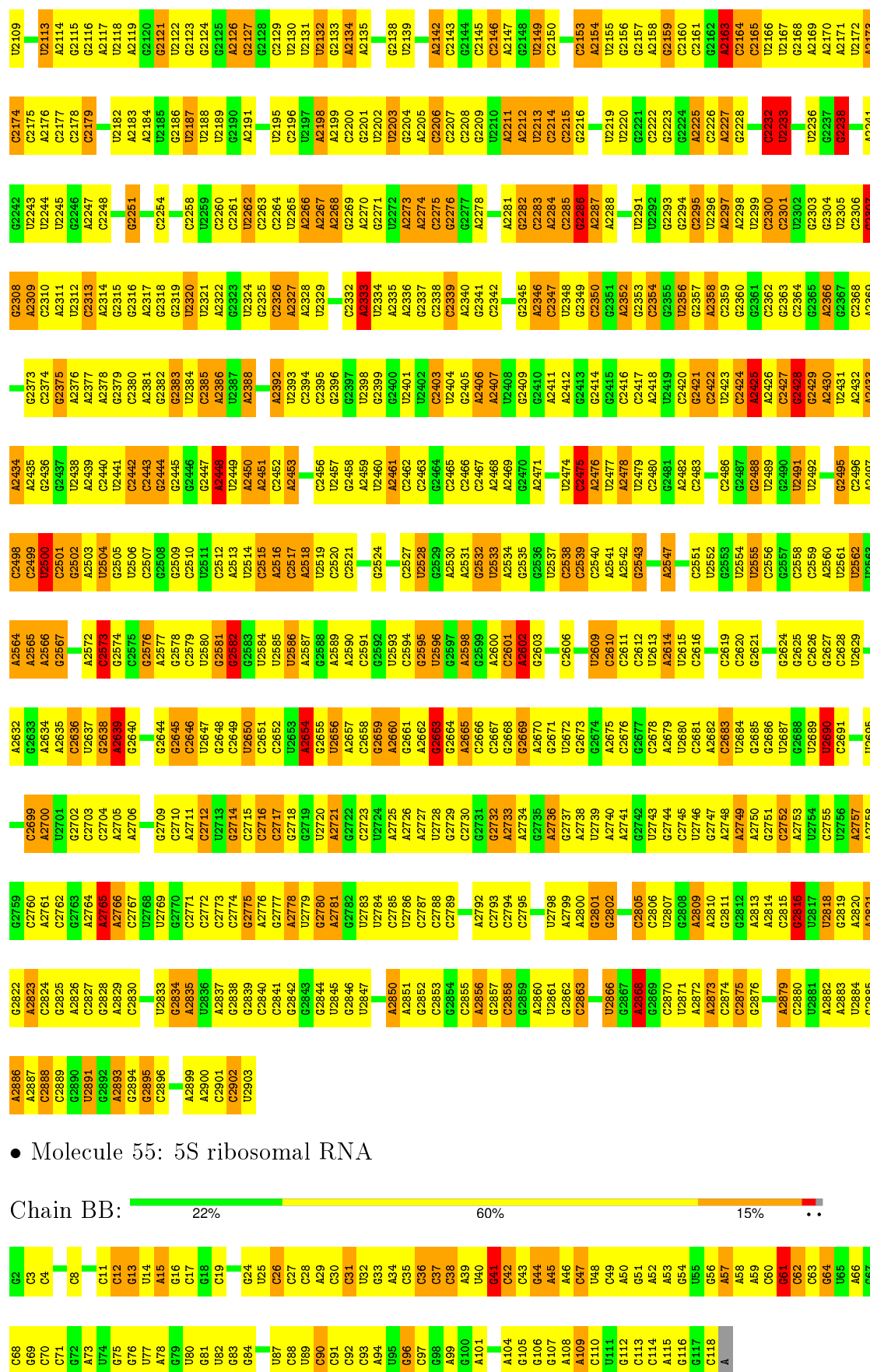


- Molecule 54: 23S ribosomal RNA

Chain BA:  22% 51% 23% .

A1028	C964	C902	U839	C772	U710	C640	G577	U448	G317	G250	G189	A126	U62	G1
A1029	C965	C903	C840	U773	G711	U641	G578	A449	C318	A251	A190	A127	A63	G2
G1030	G904	G905	G841	G774	U714	A642	G579	U450	G319	G252	A191	C128	A64	U3
A1031	G969	A905	A844	G775	A715	A643	U580	U451	A320	C253	A192	C129	U65	U4
A1032	U970	C908	A845	A781	A716	A644	C581	A452	U321	G254	U193	C130	C66	A5
G1033	G971	A909	U846	A782	A717	C645	A582	A453	A322	A255	G194	A131	U67	A6
G1034	G972	A910	U847	A783	G717	U646	A583	A454	C323	A256	A195	G132	G68	G7
U1035	A973	A911	C848	G784	A718	G647	C584	C455	A324	C257	A196	U133	G69	G8
G1038	G974	U912	U849	G785	C719	C650	G585	C456	G327	G260	C198	G134	G70	G9
A1039	A975	U913	A850	C786	A720	U653	A586	A457	U328	G261	A199	U138	A71	A10
A1040	G976	C915	C851	C787	A722	A654	C587	U459	G329	A262	U200	U139	U72	C11
C1043	A979	G916	U852	A788	C723	U655	A590	A460	A330	G263	C201	A140	A73	U12
C1044	A980	A917	C853	A789	U724	A855	U591	C461	C331	C264	U202	G141	A74	U13
C1045	A981	A918	G854	U790	G726	G856	A592	C462	A332	A265	A203	A142	G75	A14
A1046	A982	A919	C855	C791	A727	U658	C595	U463	G333	G266	A204	A143	C76	G15
C1047	A983	U919	C856	A792	A728	C659	U596	U464	C334	C267	G205	A144	U78	G16
A1048	A984	A920	C857	A793	G728	C660	U597	A466	C335	C268	U206	A145	G17	U18
C1049	A985	C921	G858	A794	G729	A661	C598	A467	C336	C269	A207	A146	C79	A19
A1050	C986	G922	G859	C795	A730	G662	U599	A468	C337	A270	C208	C147	U82	C20
G1051	C987	G923	U860	C796	C732	A663	G600	U469	G338	G271	C209	U148	A83	A21
C1052	A988	A925	G862	G733	G733	A666	C601	A470	U339	A272	C210	A149	A84	C22
C1053	G989	G926	A863	G801	A734	U667	G602	A471	C341	C274	C211	U150	G85	G23
A1054	A990	A927	C864	A802	A735	A668	A603	A472	A342	C275	A213	C151	G86	G24
G1055	C991	A928	C865	U803	C736	G669	A604	A473	C343	U276	U153	U153	A89	G26
A1056	G992	U929	A866	A804	C737	A670	U606	C476	A344	G277	A216	U154	U90	G27
A1057	C993	G930	C867	G805	G738	C671	U607	A477	A345	A278	A217	U155	A91	A28
U1060	C994	U931	C868	C906	A739	C672	A608	A478	A346	A279	A218	U156	U92	U29
U1061	C995	U932	U871	U807	C740	C673	A609	A479	A347	U280	A219	C157	G93	G30
G1062	A996	A933	G872	U741	G741	G674	C610	A480	A348	C281	G220	U158	A94	C31
G1063	C997	U934	C873	A742	A742	A675	C611	A481	U349	A282	A221	G159	A95	C32
C1064	C998	C935	C874	U743	A743	A676	G612	U482	G350	G283	A222	U160	C96	C33
U1065	U999	A936	C875	G744	G744	A677	A613	A483	C351	U284	A223	U161	C97	U34
U1066	A1001	G938	C876	U745	U745	C678	A614	A484	A352	U285	U224	U162	G98	U35
A1067	U1004	A941	C877	U746	U746	C679	U615	C485	C353	U290	C225	C163	U99	C37
G1068	C1005	G942	A878	U747	G748	C680	A616	A486	A354	G291	A226	C164	U100	A38
A1069	C1006	A943	C879	G748	C748	A685	U617	C487	U357	U292	A227	A165	A101	G39
G1070	C1007	U944	G880	A749	A749	U885	G618	U488	U358	U293	C228	U166	U102	U40
C1071	A1008	G945	C881	A750	A750	U886	G619	A489	A359	A294	C229	A167	A103	C41
C1072	A1009	A946	C882	A751	A751	A689	G620	C490	G361	U296	G230	G168	A104	A42
A1073	A1010	C946	U883	A752	A752	A690	A621	A491	A362	U297	A231	G169	C105	G43
G1074	U1010	A947	C884	A753	U753	G690	G622	A492	A363	G298	G232	U170	C106	A44
C1075	G1011	C948	C885	U754	U754	C691	C623	A493	G364	U299	U234	A172	G107	G45
C1076	U1012	G949	A886	U755	U755	C692	C624	U494	U365	A300	U235	A173	G108	G46
A1077	C1013	G950	U887	G756	G756	A693	G625	A495	C366	G301	C236	U174	G110	G48
U1078	A1014	C951	C888	U757	U757	G696	A626	A496	G367	C302	C237	G175	A111	C47
C1079	U1015	G952	C889	G758	G758	G697	A627	A497	U368	C303	C238	A176	U50	C51
A1080	U1016	G953	C890	G759	G759	C698	G628	A498	A369	C304	C239	G177	C115	G51
U1081	U1017	G954	C891	U760	A761	A699	G629	G500	U369	C305	C240	G178	C116	A52
U1082	U1018	U955	A892	A762	U762	A699	G630	A501	G370	U306	G241	G179	G117	A53
U1083	A1020	G956	C893	U763	G763	U702	A632	A502	A371	G307	A242	G180	A118	G54
A1084	A1021	C957	U894	A764	U764	G703	A633	A503	G372	G308	G243	G181	A119	G55
A1085	U1022	U958	C895	A765	C765	A704	C634	A504	U373	A309	U243	A182	U120	A56
A1086	G1023	G959	C896	U766	U766	G705	A635	A505	A374	A310	G244	A183	G121	C57
G1087	G1024	A960	C897	U767	U767	A706	G636	A506	G375	A311	G245	C184	G122	G58
A1088	A1025	C961	C898	G768	G768	G707	A637	A507	G376	C314	G246	G187	G123	U59
A1089	G1026	G962	C899	G769	G769	G708	A638	A508	C377	G315	G247	G188	G124	G60
A1090	A1027	U963	C901	G770	G770	U709	U639	C510	G379	C316	C248	G188	G125	G61


C2045	G1980	A1789	C1728	A1665	U1602	G1540	G1478	C1417	G1346	A1285	C1221	G1154	G1091
G2046	A1981	C1790	U1729	G1666	A1603	C1541	G1479	C1418	A1347	A1286	C1221	A1154	C1092
C2047	U1982	A1791	G1730	G1667	C1604	C1542	U1480	A1419	C1348	A1287	U1224	A1155	G1093
G2048	U1855	G1792	G1731	A1668	C1605	G1543	U1481	A1420	C1349	G1288	G1225	G1157	U1094
C2049	G1857	C1793	C1732	A1669	C1606	A1544	G1482	G1421	C1350	C1289	G1226	A1095	A1096
G2050	A1858	A1794	G1733	C1670	C1607	A1545	G1483	G1422	C1351	C1290	G1227	U1158	A1097
A2051	U1859	C1795	G1734	A1671	A1608	G1546	U1484	G1423	U1352	G1291	G1228	G1160	U1097
A2052	U1926	U1796	A1735	A1672	A1609	C1547	U1485	G1424	A1353	G1292	C1229	C1161	A1098
G2053	A1927	U1797	U1736	G1673	A1610	A1548	U1486	U1425	A1354	G1293	C1230	G1162	G1099
C2054	U1865	G1798	G1737	A1674	C1611	A1549	U1487	G1426	G1355	U1294	U1231	G1163	C1100
A2055	A1866	G1799	G1738	C1675	C1612	C1550	U1488	A1426	G1356	C1295	G1232	G1164	U1101
A2056	G1867	C1800	A1739	A1676	G1613	A1551	G1489	C1428	G1357	G1296	C1233	A1165	C1102
A2057	U1868	A1801	G1740	A1677	A1614	A1552	A1490	G1429	G1358	C1297	U1234	G1166	A1103
A2058	G1869	A1802	C1741	A1678	C1615	A1553	G1491	G1430	A1359	C1298	G1235	C1167	C1104
A2059	C1870	U1803	U1742	A1679	A1616	U1554	G1492	A1431	C1362	G1299	G1236	G1168	U1105
A2060	A1871	C1804	G1743	U1680	C1617	C1555	C1493	G1432	G1300	G1300	A1237	A1169	G1106
A2061	A1872	A1805	A1744	G1681	A1618	C1556	A1494	A1433	A1363	A1301	G1238	C1170	G1107
A2062	G1873	C1806	A1745	G1682	G1619	C1557	A1495	A1434	G1364	A1302	G1239	C1171	U1108
C2063	U1874	A1807	A1746	U1683	G1620	C1558	A1496	G1435	A1365	G1303	U1240	C1172	U1109
C2064	G1875	A1808	U1747	G1684	U1624	U1559	U1497	G1436	A1366	A1304	U1241	G1110	G1110
C2065	A1876	A1809	C1748	C1685	C1625	U1562	C1498	A1437	A1367	C1305	U1242	A1175	A1111
C2066	G1877	A1810	A1749	C1686	A1626	U1562	C1499	U1438	G1368	A1307	A1244	U1176	G1112
C2067	U1878	G1811	U1750	C1687	U1627	U1563	A1502	U1441	G1371	C1308	U1245	G1177	G1113
C2068	G1879	U1812	G1752	A1689	U1628	C1564	A1503	U1442	U1372	G1311	A1247	U1188	C1114
A2069	U1880	G1813	G1753	A1690	A1630	C1565	A1504	U1443	A1373	U1312	G1248	G1185	C1115
A2070	C1881	U1814	A1754	C1691	U1631	A1566	A1505	U1444	G1374	U1313	U1249	G1186	G1116
A2071	U1882	A1815	G1755	C1692	A1632	G1567	U1506	G1444	U1375	C1314	G1250	G1187	C1121
C2072	U1883	C1816	G1756	G1695	G1633	G1568	C1507	G1445	C1376	C1315	G1252	U1188	C1122
C2073	G1884	G1817	A1757	G1696	A1634	A1569	A1508	G1446	G1377	U1316	A1253	A1189	C1123
U2074	A1885	U1818	U1758	G1697	U1635	A1570	A1509	C1447	A1378	G1317	A1254	G1190	G1124
U2075	U1886	A1819	A1759	A1698	U1636	A1571	G1510	G1448	A1379	U1318	U1255	G1191	G1125
U2076	C1887	U1820	C1760	G1699	A1637	A1572	C1512	C1451	A1383	C1320	G1256	G1192	G1126
A2077	G1888	A1821	C1761	G1700	C1638	C1574	A1453	A1452	A1384	A1321	C1257	G1193	A1126
C2078	A1889	G1822	A1762	A1701	U1639	U1575	C1518	A1454	A1385	A1322	U1258	A1194	G1128
A2079	U1890	U1823	G1763	G1702	A1640	C1576	G1519	G1455	C1386	C1323	G1259	G1195	A1129
C2080	G1891	G1824	C1764	G1703	A1641	C1577	C1518	G1456	A1387	G1324	A1260	G1196	U1130
A2081	C1892	U1825	U1765	C1704	G1642	C1578	C1519	U1457	U1391	U1326	A1262	U1199	G1131
A2082	C1893	G1826	G1766	A1705	G1643	U1579	U1520	U1458	A1392	A1327	A1263	C1200	A1133
G2083	C1894	A1827	C1767	C1706	C1644	A1579	G1521	U1459	A1393	A1328	A1264	U1201	A1134
C2084	C1895	U1828	U1768	G1707	G1645	A1580	U1522	U1460	U1394	U1329	A1265	G1135	G1136
U2085	A1899	C1830	G1770	C1708	G1646	C1581	C1526	C1461	A1395	C1330	G1266	A1204	G1137
U2086	A1900	C1831	G1771	U1709	U1647	A1582	G1527	C1462	U1396	G1332	A1267	G1205	U1140
G2087	A1901	C1832	A1772	G1710	U1648	A1583	G1528	C1463	U1397	G1333	A1268	G1206	U1141
C2088	C1902	C1833	A1773	U1711	G1649	U1584	G1529	U1464	C1398	G1334	C1270	G1207	A1142
A2090	U1903	C1836	C1774	U1712	A1650	C1585	A1528	U1465	U1402	A1336	A1272	G1210	A1143
C2091	C1905	C1837	U1775	A1713	G1651	A1586	G1527	U1466	A1403	U1273	A1273	C1211	A1144
U2092	U1908	G1839	U1777	G1715	A1652	U1587	G1527	U1467	U1404	G1338	A1274	C1212	C1145
C2093	C1909	U1841	U1778	U1716	A1654	C1588	U1528	U1467	U1405	G1339	A1275	A1213	C1146
A2094	G1910	C1842	U1779	G1717	C1655	C1592	G1529	U1468	U1406	U1340	A1276	A1214	A1147
C2095	U1911	C1843	U1780	G1718	C1656	A1591	U1529	U1469	A1413	A1342	C1278	G1215	C1150
A2096	G1912	C1844	U1781	G1719	U1657	A1592	G1530	U1470	U1414	G1343	U1283	G1217	A1151
C2097	A1913	C1845	U1782	C1719	C1658	C1593	A1532	G1471	U1415	U1344	G1283	G1218	C1152
G2100	G1914	G1846	A1783	U1722	G1659	A1594	C1533	G1472	U1416	G1341	C1278	G1219	C1153
A2101	C1915	U1847	A1784	A1723	G1660	A1597	U1534	C1473	A1413	A1342	C1278	G1219	C1153
G2102	U1915	G1848	A1785	G1724	G1661	A1598	U1535	U1474	A1413	A1342	C1278	G1219	C1153
C2103	A1916	A1847	A1786	G1725	G1662	A1599	U1536	U1475	U1414	A1343	G1283	G1219	C1153
C2104	U1917	U1848	A1787	U1726	G1663	A1600	U1537	U1476	U1415	U1344	G1283	G1219	C1153
A2108	C2042	C2043	A1787	G1726	G1663	A1601	U1538	A1477	G1416	C1345	A1284	G1219	C1153



- Molecule 55: 5S ribosomal RNA

Chain BB: 

● Molecule 56: 50S ribosomal protein L1

Chain B5:  88% 7% 5%



## 4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	5656	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	4k CCD camera (TVIPS)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, FME, ACE, H2U, CM0, 6MZ, NH2, 4SU, 7MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	AB	0.69	0/1736	1.04	13/2340 (0.6%)
10	AK	0.73	0/894	1.19	10/1207 (0.8%)
11	AL	0.74	0/969	1.23	16/1300 (1.2%)
12	AM	0.74	0/884	1.35	18/1181 (1.5%)
13	AN	0.77	0/817	1.35	14/1088 (1.3%)
14	AO	0.70	0/722	1.26	10/964 (1.0%)
15	AP	0.75	0/648	1.16	7/870 (0.8%)
16	AQ	0.69	0/658	1.15	6/883 (0.7%)
17	AR	0.78	0/463	1.19	6/623 (1.0%)
18	AS	0.74	0/653	1.23	6/879 (0.7%)
19	AT	0.68	0/672	1.06	6/890 (0.7%)
2	AC	0.71	0/1651	1.12	15/2225 (0.7%)
20	AU	0.83	0/431	1.55	6/572 (1.0%)
21	AA	1.57	0/36759	2.22	1953/57346 (3.4%)
22	A1	1.59	0/1668	2.19	92/2595 (3.5%)
23	A2	1.54	0/343	2.27	23/531 (4.3%)
24	A3	1.58	1/1722 (0.1%)	2.19	93/2685 (3.5%)
25	BC	0.72	0/2121	1.26	26/2852 (0.9%)
26	BD	0.66	0/1586	1.19	13/2134 (0.6%)
27	BE	0.66	0/1571	1.13	10/2113 (0.5%)
28	BF	0.73	0/1444	1.17	10/1937 (0.5%)
29	BG	0.68	0/1343	1.18	11/1816 (0.6%)
3	AD	0.75	0/1665	1.23	21/2227 (0.9%)
30	BH	0.64	0/1122	1.12	5/1515 (0.3%)
31	BI	0.63	0/1046	1.07	4/1410 (0.3%)
32	BJ	0.70	0/1152	1.17	10/1551 (0.6%)
33	BK	0.69	0/947	1.22	10/1268 (0.8%)
34	BL	0.74	0/1054	1.31	10/1403 (0.7%)
35	BM	0.74	0/1093	1.23	12/1460 (0.8%)
36	BN	0.75	0/973	1.41	17/1301 (1.3%)
37	BO	0.71	0/902	1.24	11/1209 (0.9%)
38	BP	0.72	0/929	1.32	15/1242 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.77	0/960	1.34	18/1278 (1.4%)
4	AE	0.68	0/1119	1.06	8/1506 (0.5%)
40	BR	0.68	0/829	1.10	4/1107 (0.4%)
41	BS	0.64	0/864	1.15	6/1156 (0.5%)
42	BT	0.64	0/744	1.22	7/994 (0.7%)
43	BU	0.68	0/787	1.16	6/1051 (0.6%)
44	BV	0.68	0/766	1.19	8/1025 (0.8%)
45	BW	0.75	0/604	1.28	6/799 (0.8%)
46	BX	0.74	0/635	1.38	9/848 (1.1%)
47	BY	0.66	0/510	1.16	5/677 (0.7%)
48	BZ	0.69	0/453	1.24	3/605 (0.5%)
49	B0	0.73	0/450	1.24	5/599 (0.8%)
5	AF	0.71	0/835	1.13	8/1128 (0.7%)
50	B1	0.69	0/417	1.04	2/556 (0.4%)
51	B2	0.81	0/380	1.47	11/498 (2.2%)
52	B3	0.72	0/513	1.20	6/676 (0.9%)
53	B4	0.67	0/303	1.22	4/397 (1.0%)
54	BA	1.44	16/69796 (0.0%)	2.22	4183/108888 (3.8%)
55	BB	1.46	0/2800	2.16	142/4367 (3.3%)
56	B5	0.63	0/1673	1.11	10/2255 (0.4%)
6	AG	0.73	0/1188	1.19	15/1593 (0.9%)
7	AH	0.69	0/989	1.09	10/1326 (0.8%)
8	AI	0.78	0/1035	1.20	10/1377 (0.7%)
9	AJ	0.72	0/797	1.23	13/1079 (1.2%)
All	All	1.31	17/160085 (0.0%)	2.00	6978/239402 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	AL	0	1
18	AS	0	1
21	AA	0	346
22	A1	0	12
23	A2	0	4
24	A3	0	13
3	AD	0	2
38	BP	0	1
4	AE	0	1
50	B1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	BA	0	647
55	BB	0	19
56	B5	0	1
8	AI	0	1
9	AJ	0	1
All	All	0	1051

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1784	A	N3-C4	5.88	1.38	1.34
54	BA	2405	G	C2-N2	-5.24	1.29	1.34
54	BA	901	C	C4-N4	-5.22	1.29	1.33
54	BA	192	C	C4-N4	-5.21	1.29	1.33
54	BA	2332	C	C4-N4	-5.19	1.29	1.33

The worst 5 of 6978 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2063	C	N3-C2-O2	-17.09	109.94	121.90
54	BA	614	A	O4'-C1'-N9	14.96	120.17	108.20
22	A1	73	A	N1-C6-N6	-14.17	110.10	118.60
54	BA	548	G	O4'-C1'-N9	12.93	118.55	108.20
54	BA	2114	A	N1-C6-N6	-12.72	110.97	118.60

There are no chirality outliers.

5 of 1051 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	75	TYR	Sidechain
3	AD	96	ARG	Sidechain
4	AE	53	ARG	Sidechain
8	AI	129	ARG	Sidechain
9	AJ	72	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	1	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	3	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	3	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	841	0	0
25	BC	2083	0	2157	1	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	1	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	1	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31298	6	0
55	BB	2504	0	1269	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99612	17	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 17 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AL:69:GLU:H	11:AL:106:VAL:HG13	1.75	0.52
54:BA:1349:C:N4	54:BA:1383:A:H61	2.11	0.49
54:BA:1324:G:H3'	54:BA:1325:U:H5''	1.97	0.46
4:AE:88:HIS:CG	4:AE:89:THR:H	2.32	0.45
33:BK:111:LYS:HE3	33:BK:112:PHE:CZ	2.52	0.45

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	201 (92%)	15 (7%)	2 (1%)	21	67
2	AC	205/208 (99%)	190 (93%)	9 (4%)	6 (3%)	6	43
3	AD	203/206 (98%)	191 (94%)	9 (4%)	3 (2%)	13	57
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	9	51
5	AF	99/101 (98%)	87 (88%)	7 (7%)	5 (5%)	2	30
6	AG	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	4	35
7	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	24	69
8	AI	126/128 (98%)	110 (87%)	15 (12%)	1 (1%)	24	69
9	AJ	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	3	35
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	21	67
11	AL	121/124 (98%)	110 (91%)	9 (7%)	2 (2%)	11	55
12	AM	112/115 (97%)	92 (82%)	16 (14%)	4 (4%)	4	38
13	AN	98/101 (97%)	92 (94%)	4 (4%)	2 (2%)	9	51
14	AO	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	2	27
15	AP	79/81 (98%)	69 (87%)	6 (8%)	4 (5%)	2	30
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	11	53
18	AS	79/81 (98%)	69 (87%)	7 (9%)	3 (4%)	4	37
19	AT	84/86 (98%)	80 (95%)	3 (4%)	1 (1%)	16	61
20	AU	51/53 (96%)	38 (74%)	9 (18%)	4 (8%)	1	20
25	BC	270/273 (99%)	235 (87%)	27 (10%)	8 (3%)	5	42
26	BD	207/209 (99%)	185 (89%)	16 (8%)	6 (3%)	6	43
27	BE	199/201 (99%)	180 (90%)	11 (6%)	8 (4%)	4	35
28	BF	176/179 (98%)	157 (89%)	13 (7%)	6 (3%)	5	40
29	BG	174/177 (98%)	155 (89%)	18 (10%)	1 (1%)	30	74
30	BH	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	9	51
31	BI	139/142 (98%)	129 (93%)	9 (6%)	1 (1%)	26	71
32	BJ	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	6	43
33	BK	121/123 (98%)	103 (85%)	13 (11%)	5 (4%)	3	35
34	BL	141/144 (98%)	109 (77%)	24 (17%)	8 (6%)	2	28
35	BM	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	13	57
36	BN	119/121 (98%)	105 (88%)	13 (11%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	21	67
38	BP	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	4	38
39	BQ	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	7	45
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	9	51
41	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	10	52
42	BT	92/94 (98%)	79 (86%)	9 (10%)	4 (4%)	3	34
43	BU	101/104 (97%)	87 (86%)	9 (9%)	5 (5%)	3	31
44	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
45	BW	78/80 (98%)	54 (69%)	15 (19%)	9 (12%)	0	9
46	BX	75/79 (95%)	64 (85%)	8 (11%)	3 (4%)	4	35
47	BY	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	12	56
48	BZ	56/59 (95%)	52 (93%)	1 (2%)	3 (5%)	2	29
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2	28
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8	48
52	B3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5	41
53	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	44
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5259 (90%)	459 (8%)	158 (3%)	10	45

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AM	107	THR
14	AO	45	HIS
20	AU	9	GLU
20	AU	37	TYR
25	BC	181	ARG

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	175 (97%)	5 (3%)	51	78
2	AC	170/171 (99%)	169 (99%)	1 (1%)	90	95
3	AD	172/173 (99%)	172 (100%)	0	100	100
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	119 (97%)	4 (3%)	45	76
7	AH	104/105 (99%)	103 (99%)	1 (1%)	82	92
8	AI	105/105 (100%)	103 (98%)	2 (2%)	65	86
9	AJ	86/86 (100%)	85 (99%)	1 (1%)	78	90
10	AK	90/90 (100%)	85 (94%)	5 (6%)	26	62
11	AL	103/104 (99%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	89 (98%)	2 (2%)	60	83
13	AN	83/84 (99%)	82 (99%)	1 (1%)	78	90
14	AO	76/77 (99%)	75 (99%)	1 (1%)	76	89
15	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	52	79
17	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
18	AS	70/70 (100%)	68 (97%)	2 (3%)	50	78
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	41 (93%)	3 (7%)	20	57
25	BC	216/217 (100%)	211 (98%)	5 (2%)	58	83
26	BD	164/164 (100%)	161 (98%)	3 (2%)	66	87
27	BE	165/165 (100%)	163 (99%)	2 (1%)	78	90
28	BF	149/150 (99%)	145 (97%)	4 (3%)	52	79
29	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
30	BH	114/114 (100%)	113 (99%)	1 (1%)	84	93
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	100 (97%)	3 (3%)	50	78
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	108 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	82	92
37	BO	86/87 (99%)	84 (98%)	2 (2%)	58	83
38	BP	99/100 (99%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	91 (98%)	2 (2%)	60	83
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	80 (96%)	3 (4%)	42	74
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	54 (92%)	5 (8%)	13	48
46	BX	67/68 (98%)	66 (98%)	1 (2%)	72	88
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	61	84
49	B0	47/48 (98%)	47 (100%)	0	100	100
50	B1	45/45 (100%)	43 (96%)	2 (4%)	35	69
51	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	47 (92%)	4 (8%)	16	51
53	B4	34/34 (100%)	33 (97%)	1 (3%)	50	78
56	B5	173/181 (96%)	171 (99%)	2 (1%)	78	90
All	All	4842/4870 (99%)	4755 (98%)	87 (2%)	69	87

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	BD	2	ILE
29	BG	2	ARG
52	B3	23	HIS
26	BD	70	LYS
28	BF	6	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
26	BD	173	GLN

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Mol	Chain	Res	Type
27	BE	165	HIS
50	B1	18	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	244 (15%)	92 (6%)
22	A1	73/76 (96%)	11 (15%)	2 (2%)
23	A2	14/15 (93%)	6 (42%)	3 (21%)
24	A3	77/77 (100%)	18 (23%)	8 (10%)
54	BA	2902/2903 (99%)	468 (16%)	130 (4%)
55	BB	116/118 (98%)	17 (14%)	3 (2%)
All	All	4711/4722 (99%)	764 (16%)	238 (5%)

5 of 764 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	10	A
21	AA	13	U
21	AA	14	U

5 of 238 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	60	G
54	BA	625	G
54	BA	2373	G
54	BA	101	A
54	BA	374	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected



value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	CM0	A1	34	22,23	15,26,27	1.84	3 (20%)	18,37,40	3.28	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.89	0	15,36,39	1.08	1 (6%)
22	7MG	A1	46	22	20,26,27	2.17	3 (15%)	23,39,42	2.01	2 (8%)
22	5MU	A1	54	22	13,22,23	1.13	1 (7%)	16,32,35	4.60	2 (12%)
22	PSU	A1	55	22	15,21,22	0.99	0	16,30,33	3.28	4 (25%)
22	4SU	A1	7	22	12,21,22	0.91	0	15,30,33	2.18	2 (13%)
24	H2U	A3	21	24	17,21,22	1.40	2 (11%)	23,30,33	1.30	3 (13%)
24	OMC	A3	33	24	15,22,23	1.07	0	20,31,34	0.70	0
24	5MU	A3	55	24	13,22,23	1.07	1 (7%)	16,32,35	4.73	2 (12%)
24	PSU	A3	56	24	15,21,22	1.07	0	16,30,33	3.38	4 (25%)
24	4SU	A3	8	24	12,21,22	1.06	1 (8%)	15,30,33	2.23	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	22,23	-	0/6/30/31	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/3/25/26	0/2/2/2
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/3/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/5/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/3/25/26	0/2/2/2
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/3/25/26	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.15	1.33	1.45
22	A1	34	CM0	O5-C5	-6.00	1.25	1.37
24	A3	21	H2U	C4-N3	-3.41	1.32	1.37
24	A3	21	H2U	C2-N3	-3.01	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N7	-2.80	1.30	1.43

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	55	5MU	C5-C4-N3	-12.88	114.54	125.35
22	A1	54	5MU	C5-C4-N3	-12.70	114.69	125.35
24	A3	8	4SU	C5-C4-N3	-7.86	115.23	123.56
22	A1	7	4SU	C5-C4-N3	-7.48	115.62	123.56
22	A1	46	7MG	C5-C6-N1	-6.47	113.75	123.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	VAL	A1	101	58,22	5,6,7	0.51	0	5,7,9	1.13	0
58	FME	BA	3001	57	8,9,10	0.81	0	5,9,11	1.52	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	58,22	-	0/4/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
58	BA	3001	FME	O1-CN-N	-2.49	120.98	124.80
58	BA	3001	FME	O-C-CA	-2.14	119.84	125.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.